

PDE NOZZLE OPTIMIZATION USING A GENETIC ALGORITHM

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ABSTRACT

Genetic algorithms, which simulate evolution in natural systems, have been used to find solutions to optimization problems that seem intractable to standard approaches. In this study, the feasibility of using a GA to find an optimum, fixed profile nozzle for a pulse detonation engine (PDE) is demonstrated. The objective was to maximize impulse during the detonation wave passage and blow-down phases of operation. Impulse of each profile variant was obtained by using the CFD code *Mozart/2.0* to simulate the transient flow. After 7 generations, the method has identified a nozzle profile that certainly is a candidate for optimum solution. The constraints on the generality of this possible solution remain to be clarified.

INTRODUCTION

Transient flow fields obtained in pulse detonation engines (PDE) preclude traditional analytic methods of nozzle design, such as the Rao method or method of characteristics. Quasi-steady blow-down analysis can provide an estimate for expansion ratio but nothing about nozzle profile; also the quasi-steady assumption is of doubtful validity. It is hard to conceive of any extension or other direct analytical approach that might be satisfactory. This leaves search methods: search for the best configuration among the possibilities.

Genetic algorithms are adaptive search algorithms. Over many generations, given an inherent source of genetic variation, natural populations evolve according to the principles of natural selection and 'survival of the fittest' first clearly stated by Darwin in *The Origin of Species*. By mimicking this process, GAs are able to evolve solutions to more mundane problems involving searches for global maxima on convoluted solution spaces. J. Holland, who in 1975 was the first to rigorously lay down the basic principles, demonstrated that GAs combine exploration of the solution space and exploitation of previously visited points simultaneously and in the best way, at least theoretically.^[6]

GAs are an element of the *soft computing* techniques for solving complex problems with system uncertainty coming into use in the design of aerospace control systems, structures and components^[1,2,3]. Other applications include: (1) the design and optimization of neural networks, used for a variety of classification problems such as pattern recognition, machine learning, image processing and expert systems^[4]; (2) numerical function optimization, a traditional research area where GAs have been shown to out-perform conventional methods on difficult, discontinuous, multimodal, noisy functions^[5]; and (3) combinatorial optimization dealing with arrangement of discrete objects or allocation of resources^[6].

Here, the population consists of diverse nozzle profile variants, each encoded in a sequence of parameters (a sequence of genes forming a chromosome). Fitness is quantified as a performance characteristic determined by CFD simulation of the transient flow through the nozzle.

EVOLUTIONARY ELEMENTS

Evolution can be seen as a two step process: First, a source of hereditary genetic variation, and second, a selection of those variants most effectively propagated to following generations. Hereditary genetic variation is brought about through two mechanisms: mutation of variants and recombination of variants through sexual reproduction.

Selection. Natural selection is understood as the differential reproduction of alternative genetic variants. Some variants may increase the chances of individuals carrying them to survive and reproduce more successfully than individuals carrying alternative variants. Such individuals are the “fittest”.

In simulation, fitness is a calculable quantity. Fitness is calculated for members of the current population (nozzle variants), and those in the top n percent are ranked as potential parents for the next generation. Selection for the breeding population is made by fitness or rank weighted, random lottery.

Recombination. Recombination of the maternal and paternal genes takes place during meiosis, a type of cell division in which the diploid (double) chromosome complement is reduced by half (haploid) to form gametes (sex cells). The essential feature is the random genetic exchange that occurs between homologous sections of maternal and paternal chromosomes and results in new genetic variants (Figure 1a).

In simulation, a chromosome section marked by randomly selected break-points in the gene sequence of the father’s chromosome is swapped for the homologous section of the mother’s chromosome. This produces two offspring whose genetic structures are conjugate recombinations of the genetic material of their parents (Figure 1b).

Mutation. Mutations are randomly occurring imperfections in DNA replication. When these occur in germ cells prior to meiosis, they can be passed on to progeny. Normally the rate of occurrence is small, maybe 4 mutations per 10^5 replications. Rarely do they introduce something new that imparts a selection advantage. Nevertheless, mutation may be the main source of material for evolutionary change.

In simulation, their main role seems to be that of a mechanism lessening the potential for premature convergence. Since it is relatively easy for diversity to be lost in a small simulation population, the mutation rate is often assumed to be many times greater than that occurring in nature, say between 4 and 10 percent.

THE PDE NOZZLE ALGORITHM

Each nozzle variant must be represented by a manageable (small) set of parameters encoding sufficient information to construct its unique profile. In this experiment, a nozzle profile is given as a nine point, cubic spline-connected curve. The radial coordinate values – axial coordinates are specified – form the parameter set that, in the genetic analogy, is a chromosome. (Axial coordinate distribution was taken from a spline representation of a proto-type, Rao derived, nozzle, typical of a nozzle showing moderately aggressive expansion, with clustering near the nozzle entrance.) The first point is fixed, both axially and radially, to mate with the detonation tube. Although we will consider variants affecting the only the last eight genes, the nine gene chromosome encodes the profile,

$$[r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8, r_9].$$

During CFD simulation of the transient flow, pressure ($p - p_\infty$) is integrated over the nozzle surface every few time steps from the instant the detonation wave enters the nozzle until a programmed stop at around .4ms when pressure in the detonation tube has relaxed sufficiently for recharging. The impulse at cut-off is taken as the nozzle's fitness value.

The *Mozart*[†] PDE model has a detonation tube length to radius ratio of 10.0 (.2 m long, .02 m radius), and a nozzle length nominally half the tube length. It is charged with a stoichiometric mixture of H₂ and O₂ at 2 atms pressure. This is also the pressure to which blowdown must relax for purge/recharge to begin. Ambient pressure is 1 atm. Computations are performed with full chemistry, inviscidly.

Mozart is initialized for its chosen charge and quiescent conditions. The nozzle is any nozzle that has the chosen grid dimensions. *Mozart* is then run. A detonation wave forms and propagates down the tube. Just as it reaches the exit plane of the tube, the run is stopped and all flow conditions, including history and thrust history files, are saved and reserved for initialization of all subsequent trials. Thereafter we can swap nozzles freely, provided they have the same grid dimensions and smoothly connect to the detonation tube, restart *Mozart* from the reserved initialization files, run until it reaches the programmed stop, and examine the nozzle's contribution to impulse. Additional details regarding the implementation of this operation will not be discussed here; they deal with procedures specific to running *Mozart*.

A diagram of the algorithm is given in figure 3. Since the present algorithm departs from tradition in using continuous variables instead of binary strings as genes, the crossover and mutation operations are slightly different than those of the earlier illustration. Figure 2 gives a geometric interpretation. The crossover operation might better be seen as a cut and translate operation. Note that the translation is exact. However, if the offspring's chromosome is mutated, translation is imperfect, determined by random trial on a

[†] *Mozart/2.0* is a research code specifically designed for transient, reacting flows. It was obtained from its developer, Jean-Luc Cambier now of MSE-TA Inc., Butte, MT. (See for instance AIAA Paper 99-2659.)

Gaussian distribution about the exact translation. (Of course there are no sharp bends in the constructed profiles.)

Each run takes roughly 45 mins. on one processor (SGI). Typically, a generation of 10 or more new members is setup and run at one time; usually, the same number of idle processors can be found on machines to which we have access.

RESULTS AND DISCUSSION

An initial population consisting of 40 members was chosen, produced by randomly generating points, subject only to the constraint that they be monotonically nondecreasing. A sample is shown in Figure 4. From this a breeding population of 10 was selected, and each successive generation consists of 10 new members. Figure 5 shows the evolution of the population. The shaded area shows nozzle impulse at cutoff, while the other curve is the maximum impulse attained (nozzle thrust can become negative before cutoff). As expected these converge; nozzle thrust is zero at cutoff for the best performance. Figure 6 shows nozzle variant 95, the best found after 7 generations. The expansion ratio of this nozzle is 3.53. For comparison, a 1-D quasi-static blowdown analysis gives an exit area ratio of around 3.5 for optimum thrust/impulse history, given an initial pressure ratio of .01 (ambient to chamber, about 20 percent higher than the maximum simulation pressure). Thereafter, little genetic diversity remained in the active population, and performance differences were minimal. The experiment was closed.

At this point, it is tempting to engage in some genetic engineering, to tamper with the genotype of the breeding population. And if the only objective were to design the optimum PDE nozzle, we would probably do so. However, in the spirit of the experiment, we restrained ourselves to better understand its flaws.

It is entirely possible to include x-locations in the gene definition. Clearly some generality is sacrificed in choosing a particular axial distribution of profile control points. Note, however, that a profile need not start expansion immediately but could merely extend the detonation tube for some distance, effectively shortening the nozzle. It did not work out this way. It would be very fortuitous for the optimum length to have been chosen by chance. More likely, any initial population profile that might have had the proper nonexpansive behavior near the entrance was linked to a poor performing downstream section and so was lost in selection, unfortunately for all time. In genetics this is called *epistasis* and refers to the fact that the effectiveness of a gene can strongly depend on the presence of other genes – a sort of nonlinearity. Unwittingly, we lost diversity quickly by picking a breeding population too small. At least for several generations, the breeding population should be large to give potentially good genes a second chance.

In summary, we should be hesitant to claim that the profile 95 is optimum. Nevertheless, the experiment was a qualified success. We have demonstrated feasibility and have

gained valuable insights into the operation and requirements of GAs in design application. We have seen how GAs explore and exploit a solution space simultaneously.

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- on the internet - <http://www.aic.nrl.navy.mil:80/galist> , check out *The Hitch-Hiker's Guide to Evolutionary Computation*.

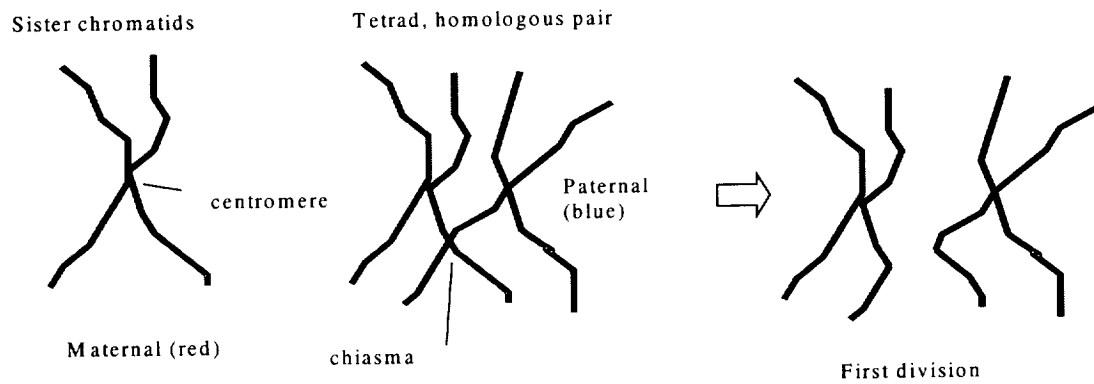


Figure 1a. Each chromosome is replicated, forming sister chromatids connected at the centromere. Maternal and paternal chromosomes come together in homologous pairs with one or more crossover sites (chiasmata).

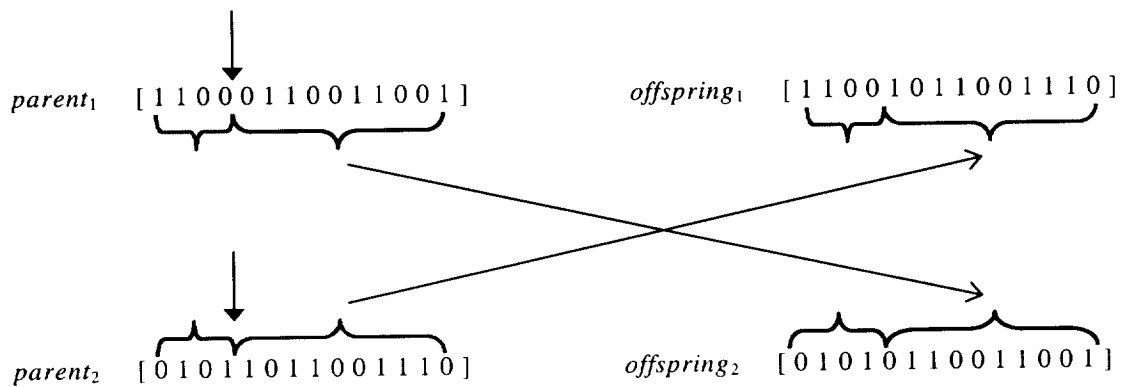


Figure 1b. Simulation. Chromosomes represented by binary strings. Crossover point marked by filled arrows.

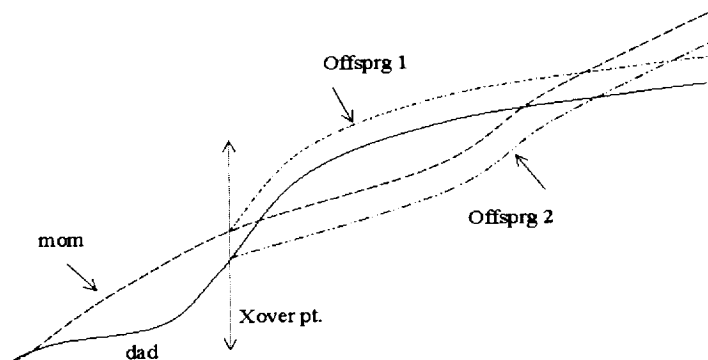


Figure 2. Crossover geometric illustration.

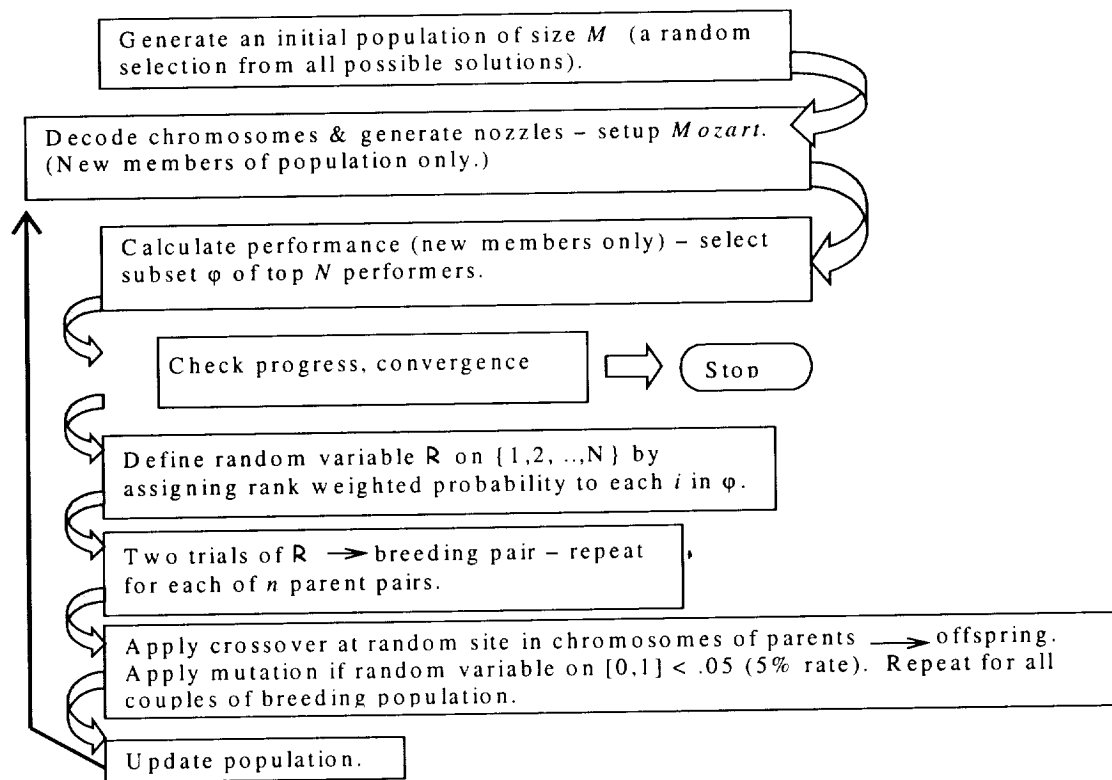


Figure 3. Algorithm schematic

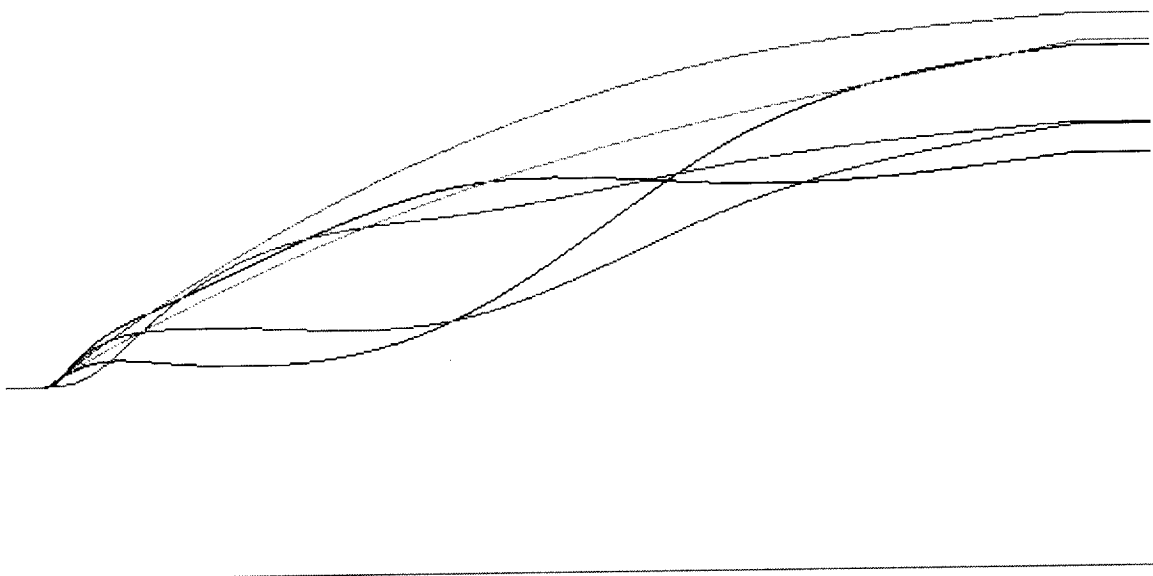


Figure 4. Sample profiles from initial population

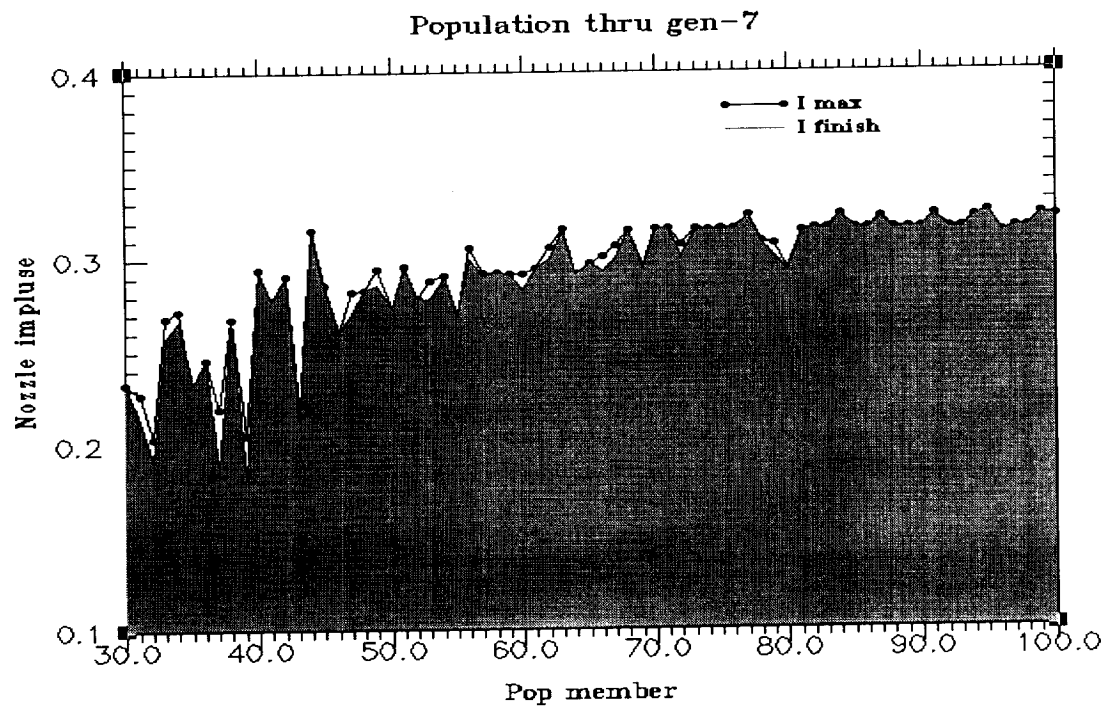


Figure 5. Evolution through generation 7

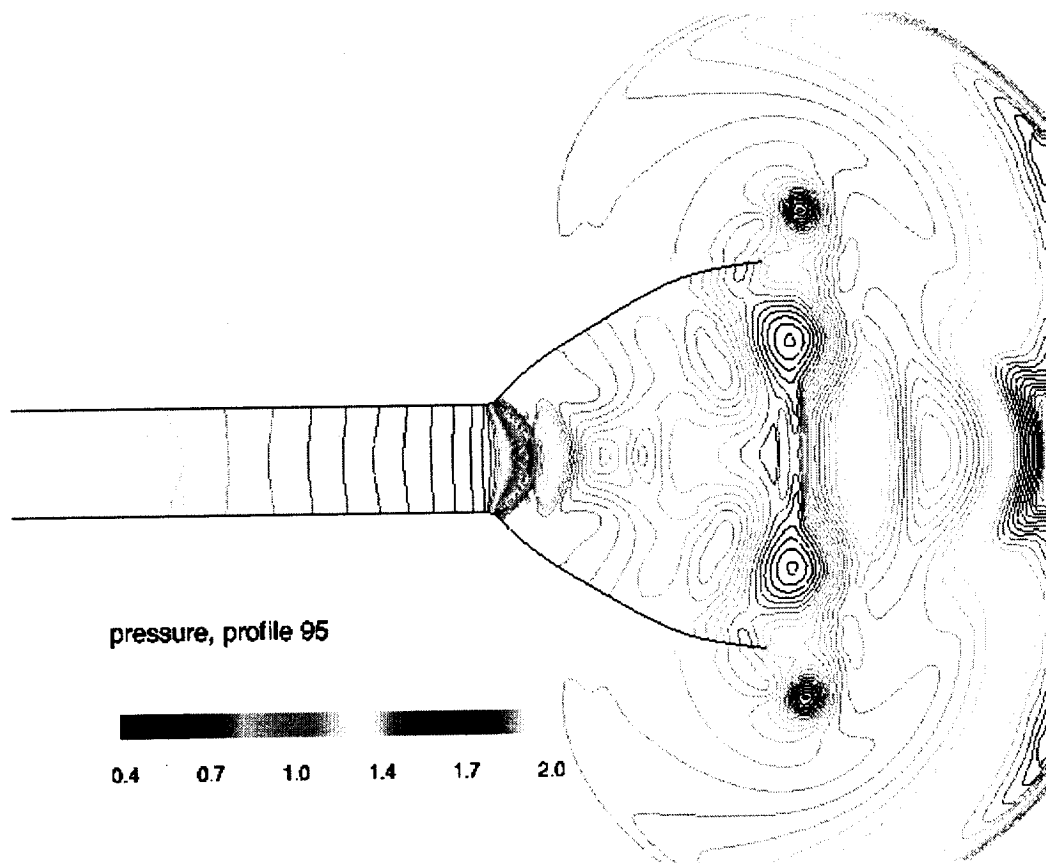


Figure 6. Tentative optimum nozzle profile (# 95) at cutoff